Numerical Modeling of 3D Electrowetting Droplet Actuation and Cooling of a Hotspot

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Abstract: Three dimensional Electrowetting on Dielectric droplet actuation have been numerically studied using COMSOL Multiphysics Two-phase Flow, Phase Field and Level Set Method. Phase Field method has been found to be more accurate in maintaining more acceptable droplet shape although Conservative Level Set method has been proved to be more effective in conserving droplet mass. A simplified single phase heat transfer conjugate convection problem for liquid droplet cooling of a hotspot has been also developed and numerically solved. Finally, this Multiphysics simulation has been compared to the experimental results.

Keywords: EWOD, Digital Microfluidics, Hotspot Cooling, COMSOL Multiphysics.

1. Introduction

In recent days, the concept of digital microfluidics (DMF) has attracted many researchers in various fields. In DMF, discrete droplets are used instead of having continuous flows which offers several advantages over continuous microfluidics. Digital microfluidics have been demonstrated as a versatile tool in a variety of applications over the past few years in different research fields; from engineering to the life sciences, including variable focus lenses, display technology, fiber optics, and lab-on-a-chip devices [1]. The use of multiple droplets acting like small microreactors offers an additional benefit besides portability and minimal operation cost due to miniaturization. As each droplet is spatially confined, a large number of experiments can be performed on a single chip surface giving rise to increased possibilities in multiplexing. In particular, efficient and cost-effective lab-on-a-chip devices are in great demand, as they allow for highly repetitive laboratory tasks to become automated [2]. Additionally, these devices do not need additional pumps or valves for liquid handling and each droplet can be addressed individually. Methods of micro-sized droplet manipulation techniques include thermo capillary actuation [3-4], dielectrophoresis [5] and electroelectrowetting [6-7]. All of these methods utilize the advantage of scalability in micro fluidics device where surface tension force becomes dominant over the body forces like gravity.

Electrowetting-on-Dielectric (EWOD) can be used as a platform for performing basic operations of DMF such as generating, splitting, merging and transporting of droplets. In EWOD, the surface tension between a liquid droplet and solid substrate is modulated by applying voltage to an electrode and thus surface can be transformed from hydrophobic to hydrophilic. Thus a droplet that is partially placed on the electrode can be moved due to asymmetric electrowetting force. Among many applications of EWOD reported in the literature [8], a novel technique is hotspot cooling for more efficient and target specific thermal management of electronics [9-10]. In this technique, a programmable array of discrete microdroplets can be used to actively cool areas of locally high heat flux known as ''hot spots.'' Heat production is an unavoidable byproduct of the operation of an electronic device. Unfortunately, excess heat can also reduce device performance and durability .As electronic systems become both smaller in size and larger in power consumption, the development of effective methods for small-scale thermal management becomes crucial. Traditionally, heat is removed from an electronic device to the surrounding environment through air-cooled heat sinks. However, liquid coolants, of which thermal conductivities are much greater than that of air, can support higher rates of heat flux. Since EWOD allows to programmably control droplet transportation, an array of discrete microdroplets can be used to cool

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hotspots specifically, efficiently and dynamically as they arise. This feature gives rise to the concept of adaptive chip cooling [9].

2. Theory

2.1 EWOD actuation

In electrowetting, an external electric potential is applied between a liquid and a solid substrate that eventually lowers the surface tension between solid and liquid due to resulting net electric charge accumulation (Fig. 1).The relation between the applied electric potential (*V*) and the resulting interfacial tension can be expressed using Lippmann Equation [13]:

$$\gamma(V) = \gamma(0) - \frac{1}{2}CV^2 \tag{1}$$

Here $\gamma(0)$ is the surface tension of the solid-liquid interface at zero potential and *c* is the capacitance per unit area, assuming the charge layer can be modeled as a symmetric Helmholtz capacitor [13].

Further the change in the interfacial tension can be approximated by the apparent contact angle change which can be expressed by Young-Lippmann Equation:

$$\mathrm{Cos}\theta = \mathrm{Cos}\theta(0) + \frac{C_d}{2\gamma}V^2 \tag{2}$$

Where γ is the liquid-gas interfacial tension, C is the capacitance per unit as before and V is the applied potential.

Now if a droplet of conductive liquid is placed partially on an activated electrode (V>0), the asymmetric radius of curvature of the droplet meniscus resulting from the different contact angle on trailing and leading meniscus of the droplet will create pressure difference on two sides of the droplets which can be realized from Young-Laplace equation :

$$\Delta P = \sigma\left(\left(\frac{\cos\theta\,(on) - \cos\theta\,(off)}{H}\right) + Kxy(off) - Kxy(on)\right) \tag{3}$$

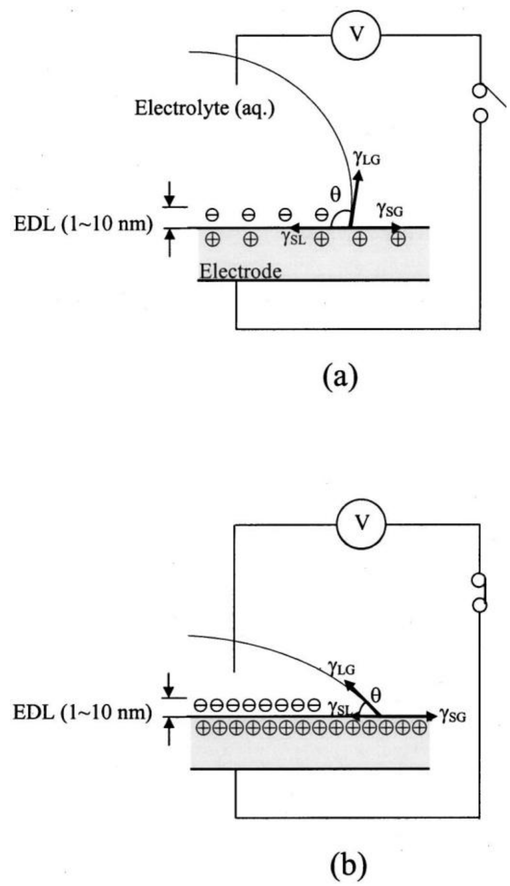

Figure 1. Principle of electrowetting. (a) No external voltage applied. Charges are distributed at the electrode-electrolyte interface, building an EDL. (b) External voltage applied. Charge density at EDL changes so that γ_{SL} and contact angle decrease or increase [13].

Where Kxy is the curvature of the droplet on x-y plane and H is the channel height for a parallel plate EWOD setup. Now this pressure difference will create a net driving force which will move the droplet (Fig. 2).

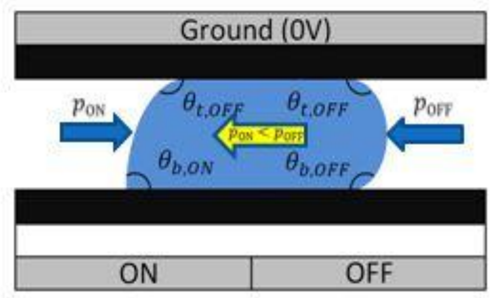

Figure 2. Pressure difference between droplet leading and trailing edge due to applied voltage on the electrode at left. As a result the droplet moves from right to left electrode. [Ref. 14]

2.2 Hotspot cooling

Because of the low cooling performance of conventional air cooling methods for thermal management of ICs, many novel cooling methods have been recently proposed by the researchers such as micro-channel cooling or evaporative cooling by piezoelectric droplet actuation. One limitation of these techniques is that, they depend on external pumps or actuators which make the system integration complicated. Also, most of these cooling methods use liquid water as coolant. But in EWOD, any electrically conductive liquid such as galinstan can be manipulated. Thermal conductivity of galinstan is known to be 65 times higher than that of water. Moreover programmability, and reconfigurability make EWOD an attractive platform of droplet based cooling, which can provide efficient and effective target specific cooling. Additionally, EWOD does not have the problem of Joule heating and the power requirement is inherently very low [10].

In a prototype of EWOD hotspot cooling chip, we can consider following components; coolant liquid reservoir, IC substrate and the hot droplet waste reservoir. The process starts with generating multiple cooled droplets from the reservoir, then transporting them across the IC surface onto the hotspots from where they transfer heat, store it and carry away heat to cool the hotspots and finally they are dispensed at the hot droplet reservoir. The micro fluidic device consists of an array of electrodes for generating and transporting droplets of coolant. Coolant droplets are sandwiched between a bottom substrate of the IC chip and a top plate. With a feedback control mechanism the dynamic hotspots can be spotted instantaneously and user defined flow paths can be programmed to transport droplets over them using 2-D electrode arrays. Thus coolant droplets can be supplied on-demand to cool the hotspots to achieve optimal thermal performance [10].

3. Problem Setup

Figure 3 illustrates the problem setup for the multiphyiscs numerical modeling. A rectangular chamber filled with air is considered to be the fluid flow domain which is supported at top and bottom by silica glass substrate. Three square shaped surfaces next to each other on the bottom plate are designed as the transporting electrodes. Another squared surface having smaller dimensions than the electrodes is positioned at the center of the middle electrode to mimic the actual “hotspot” where a constant heat flux is supplied. For reducing computational efforts only two droplets are considered as the coolant, which are transported to the middle electrode where they transfer heat with the hotspot through convection and conduction and then after staying there for some time, is transported to the third electrode. Since the channel height is very small (100µm), the z-directional curvature of the droplet is neglected and the initial droplet is considered to be cylindrical.

The following geometrical parameters are used for modeling and are listed in table 1:

Table 1 Geometrical dimensions

Parameter name	Dimension (mm)
Electrode dimension	2×2
Channel height	0.1
Hotspot dimension	0.5×0.5
Top & bottom plate thickness	0.7

4. Use of COMSOL Multiphysics

COMSOL multiphysics 5.0 has been used to simulate the problem described in section 3. To Shorten the computational time and reduce

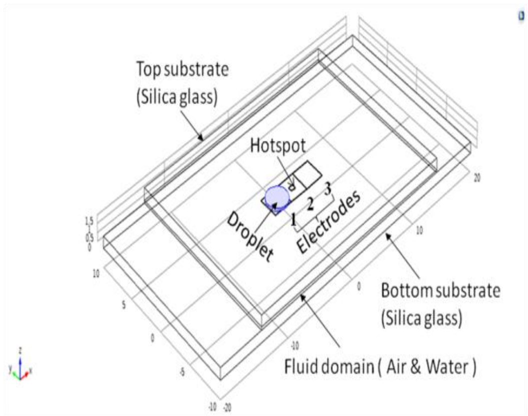

Figure 3. Setup for numerical modeling (Geometry created using COMSOL model builder tools).

computational resources, electrowetting effect in the fluid flow dynamics is directly introduced through Young-Lippman equation (Eq. 2). The fluid flow physics is therefore decoupled from the electrostatics. For solving the fluid flow dynamics, Two-Phase Flow, Phase Field and Two-Phase Flow, Level Set interface have been separately used. Simultaneously, Heat Transfer in Fluids interface is used to solve the heat transfer in both liquid and solid domain and it is coupled to the fluid flow interface to solve the coupled problem.

4.1 Governing equations

For solving the velocity and pressure field in the fluid domain, continuity (Eq. 4) and momentum (Eq. 5) equations have been solved assuming incompressible, constant property fluid and two phase flow:

$$\nabla \mathbf{u}=0 \tag{4}$$

$$\rho(\partial \mathbf{u}/\partial t+(\mathbf{u}.\nabla)\mathbf{u})=\nabla.[-p\mathrm{I}+\mu(\nabla \mathbf{u}+(\nabla \mathbf{u})^{T})]+\rho \mathbf{g} +F_{st} \tag{5}$$

Here ρ is the density of fluid, **u** is the velocity vector, μ is the fluid dynamic viscosity, t is time, p is fluid pressure, **g** is the gravitational acceleration, $\mathbf{F}_{st}$ is the surface tension force and **I** is identity matrix [14]. Further surface tension force F_{st} is defined as non-zero only at the interface using the following expression (Eq. 6):

$$F_{st}=\nabla.\sigma(\mathrm{I}-(nn)^{T})\delta \tag{6}$$

Where σ**, I,** ***n*** and δ represents co-efficient of surface tension, interface normal, identity matrix and direct delta function respectively.

Next, to track the interface of the two immiscible fluids, advection equations of the respective functions (e.g. phase field variable or level set variable) should also be solved along with the Navier-Stokes equations details of which can be found in references 11 and 12.

For solving the heat transfer problem, energy equation is solved (Eq. 7):

$$\rho Cp.\mathbf{u}.\nabla T+\rho Cp.\partial T/\partial t=\nabla.(K\boldsymbol{\nabla} T) \tag{7}$$

Further to couple the energy equation with the Navier-Stokes equations, thermal properties e.g. C_p, K and also density (ρ) have been expressed in terms of the volume fractions of the fluids and respective properties of the two-phases (Equations 8-10):

$$K=(K(water)-K(air))\times\varphi(water)+K(air) \tag{8}$$

$$Cp=(Cp(water)- Cp(air))\times\varphi(water)+ Cp(air) \tag{9}$$

$$\rho=(\rho(water)- \rho(air))\times\varphi(water)+ \rho(air) \tag{10}$$

Where K, Cp and ρ are the thermal conductivity, specific heat capacity and density of the fluid and φ is the volume fraction.

4.2 Boundary and initial conditions

In the two-phase flow, wetted wall condition and navier-slip condition have been used on the top and bottom surfaces of the fluid domains for phase field and level set method respectively. The contact angle on the bottom and top surface have been specified as that of the contact angle of water on Teflon coated surface. On the activated electrode, modified contact angle is directly calculated from Young-Lippmann equation corresponding to the applied voltage. The default no-slip condition has been maintained on the vertical boundaries. Initially no velocity, atmospheric pressure condition has been assumed and initial contact angle throughout the top and bottom surface have been taken corresponding to zero voltage. As for the heat transfer boundary conditions, boundary heat source condition has been applied on the hotspot surface. The top plate has been allowed to exchange heat with the ambient air. The side boundaries of the fluid domain are assumed to maintain outflow boundary conditions. Rest of the domain boundaries are assumed to be thermally insulated.

Table 2 Simulation parameters

Parameter name	Parameter value
Surface tension, σ	.072 [N/m]
Applied voltage, V_{ac}	150[V]
Initial contact angle,θ_o	118[degree]
Dielectric thickness, d	5[µm]
Heat Flux, q″	36.6[W/cm²]
Dielectric constant, ε_r	2.5
Convection co-efficient, h_{air}	5[W/(m.K)]
Initial temperature, T	298.15 [K]

5. Results and Discussions

First, the fluid flow simulation is carried out both using Phase Field and Level Set interface. The results are slightly different in terms of mass conservation and droplet profiles. Conservative Level Set method is found to be highly efficient in conserving mass compared to the mass conservation in phase field method. But the droplet profile is smoother in case of phase field method. As shown in figure 4, along with the unusual droplet profiles, there is some instability in case of level set method at the beginning stages of the simulation. These observations are consistent with that reported in reference 15. The computational time for level set method is significantly larger than in the case of phase field method.

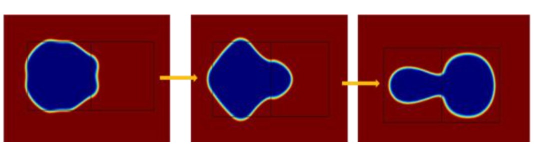

Figure 4. Droplet profiles from COMSOL simulation for level set method at different time instants. (Top view)

For Phase Field method, significant mass loss is observed. A parametric study is conducted for the numerical parameters including mobility tuning parameter (χ), tuning parameter (λ) and initial time step in order to find out their influences on mass conservation. Among these parameters, mobility tuning parameter is found to have the most dominant effect. As shown in figure 5, more mass loss is observed for lower values of the parameter. Compared to the lowest studied value of .001 of χ, the mass loss for the value of 1 was 21 % less. But this parameter also affects droplet velocity. To match our simulation results with that of the experiments performed in our group, a suitable value of χ has been finally used in the simulation with the expense of considerable mass loss. For the same physical and geometrical parameters as of the experiments already mentioned in table 1 & 2, the droplet takes almost 90 ms to complete the transition from one electrode to another as shown in figure 6 which is slightly less than the experimental case, which is about 100 ms. Unlike the level set method, phase field method is better in terms of maintaining smooth droplet profile. The comparison between the experimental and simulation results are drawn by figure 7. The slight difference between the two profiles at the same time instant can be attributed to several factors. First of all, contact angle hysteresis and contact line friction is not included in our modeling which can have significant contribution on droplet deformation leading to different droplet shapes. Also mass loss may be another factor contributing to this difference.

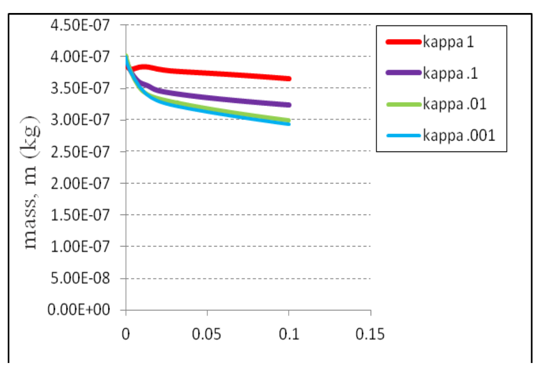

Figure 5. Effect of mobility tuning parameter on droplet mass loss for Phase Field method.

It is very important for any numerical modeling to perform mesh convergence and time convergence study for validation. Due to limitation in computational resources, those requirements are not fulfilled in the present study. However, in spite of those limitations, our numerical modeling shows quite good agreement with the experiment in terms of droplet profiles.

The cooling curve of a hotspot is obtained by solving the multipysics problem. Although in the experiments, multiple droplets need to be supplied on the hotspot to maintain a certain hotspot temperature, to reduce simulation running time only two droplets are transported over the hotspot in the entire simulation. Average hotpot temperature as a function of time has been plotted in figure 8. At the beginning, when there is no droplet over the hotspot, its temperature starts to rise. But as soon as the droplet comes over the hotspot, heat is transferred through convection from hotspot to the droplet which decreases the average hotspot temperature. During the time when droplet stays on the hotspot, heat transfer mode is conduction and gradually hotspot temperature begins to rise possibly because the droplet temperature also rises simultaneously. Further decrease of hotspot temperature is noticed during the exit of the

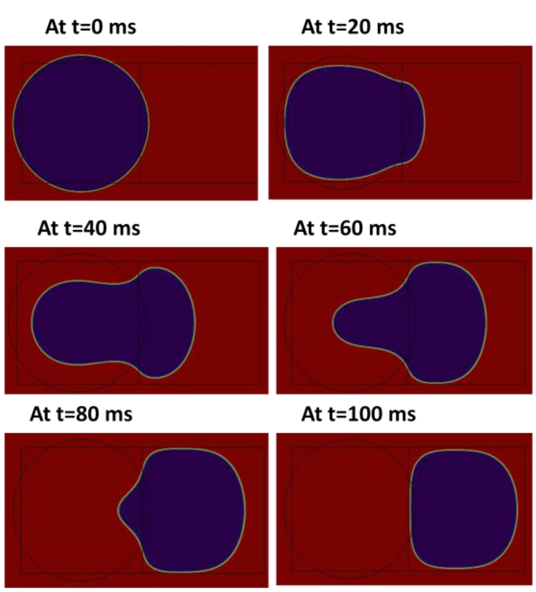

Figure 6. Droplet position in COMSOL simulation at different time instants during motion (Solved using Phase Field method). (Top view)

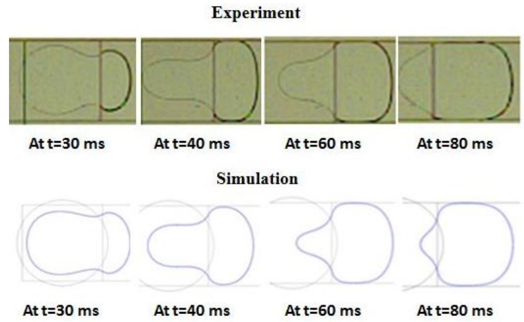

Figure 7. Comparison of droplet profiles from experiment and simulation at different time instants. (Top view)

droplet from the middle electrode which is again the contribution of convection heat transfer. In terms of pattern, simulation gives similar cooling curve as of the experiment. The difference between the two can be observed corresponding to the dwelling time of the droplet on the hotspot. In experimental case, temperature of hotspot shows a constant decrease during the dwelling time over the hotspot. The explanation for this can be drawn from experimental observations. Experimentally significant evaporation is observed at that time period and consequently there is fluid circulation inside the droplet which may have further assisted the heat exchange from the hotspot to the droplet. Marangoni convection as well as buoyancy driven convection are another phenomena that can have observable effects on the cooling curve. All of these phenomena are neglected in the simulation.

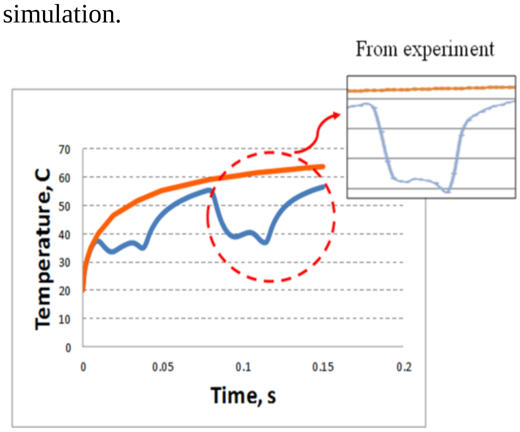

Figure 8. Average surface temperature of hotspot from simulation. The orange line is the temperature without water droplet and blue line is the temperature

with two subsequent droplets on the hotspot. In the inset, cooling curve from experiment is shown.

6. Conclusions

Three dimensional droplet motion has been simulated using COMSOL multiphysics and results have been validated with experiments which show good agreement. Multiphysics simulation has been performed to model the cooling of a hotspot by EWOD actuated droplets. Since experimentally investigating the droplet hotspot cooling requires measuring temperature and heat fluxes at numerous locations to study the cooling capacity of this technique and also to find out the parameters for optimization towards better cooling performance is both technically complicated and cumbersome, this simple coupled fluid flow and heat transfer model can be very helpful to analyze the problem with close approximation. As a future work, evaporation and Marangoni convection will be added to the model.

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